



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2025 – 12:36 PM EDT

PDB ID : 5Qsx / pdb_00005qsx
Title : PanDDA analysis group deposition – Crystal Structure of human STAG1 in complex with Z2856434812
Authors : Newman, J.A.; Katis, V.L.; Gavard, A.E.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Gileadi, O.
Deposited on : 2019-07-16
Resolution : 2.34 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

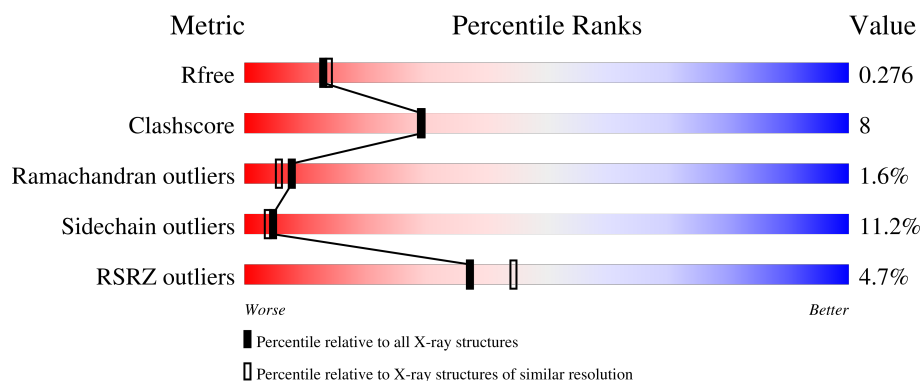
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2747 (2.36-2.32)
Clashscore	180529	2936 (2.36-2.32)
Ramachandran outliers	177936	2912 (2.36-2.32)
Sidechain outliers	177891	2912 (2.36-2.32)
RSRZ outliers	164620	2747 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	339	
1	B	339	
1	C	339	
1	D	339	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10244 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

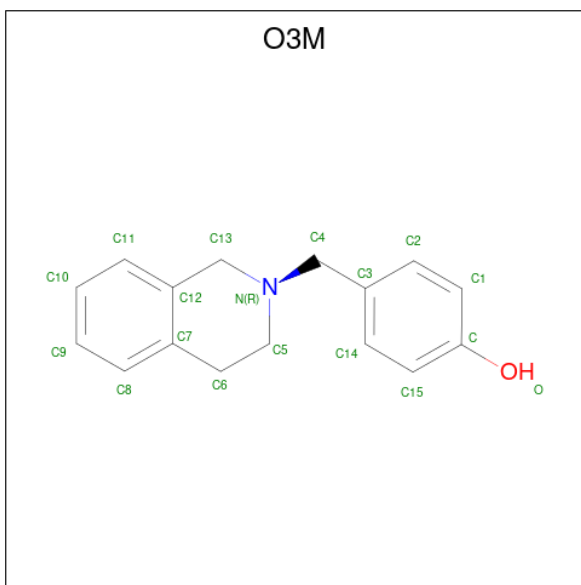
- Molecule 1 is a protein called Cohesin subunit SA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	315	Total	C	N	O	S	0	0	0
			2587	1644	447	475	21			
1	A	297	Total	C	N	O	S	0	0	0
			2433	1550	417	446	20			
1	B	298	Total	C	N	O	S	0	0	0
			2452	1566	418	448	20			
1	D	311	Total	C	N	O	S	0	0	0
			2561	1627	439	475	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	82	SER	-	expression tag	UNP Q8WVM7
C	83	MET	-	expression tag	UNP Q8WVM7
C	84	GLY	-	expression tag	UNP Q8WVM7
C	85	GLY	-	expression tag	UNP Q8WVM7
A	82	SER	-	expression tag	UNP Q8WVM7
A	83	MET	-	expression tag	UNP Q8WVM7
A	84	GLY	-	expression tag	UNP Q8WVM7
A	85	GLY	-	expression tag	UNP Q8WVM7
B	82	SER	-	expression tag	UNP Q8WVM7
B	83	MET	-	expression tag	UNP Q8WVM7
B	84	GLY	-	expression tag	UNP Q8WVM7
B	85	GLY	-	expression tag	UNP Q8WVM7
D	82	SER	-	expression tag	UNP Q8WVM7
D	83	MET	-	expression tag	UNP Q8WVM7
D	84	GLY	-	expression tag	UNP Q8WVM7
D	85	GLY	-	expression tag	UNP Q8WVM7

- Molecule 2 is 4-[(3,4-dihydroisoquinolin-2(1H)-yl)methyl]phenol (CCD ID: O3M) (formula: C₁₆H₁₇NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			18	16	1	1		
2	B	1	Total	C	N	O	0	0
			18	16	1	1		
2	D	1	Total	C	N	O	0	0
			18	16	1	1		

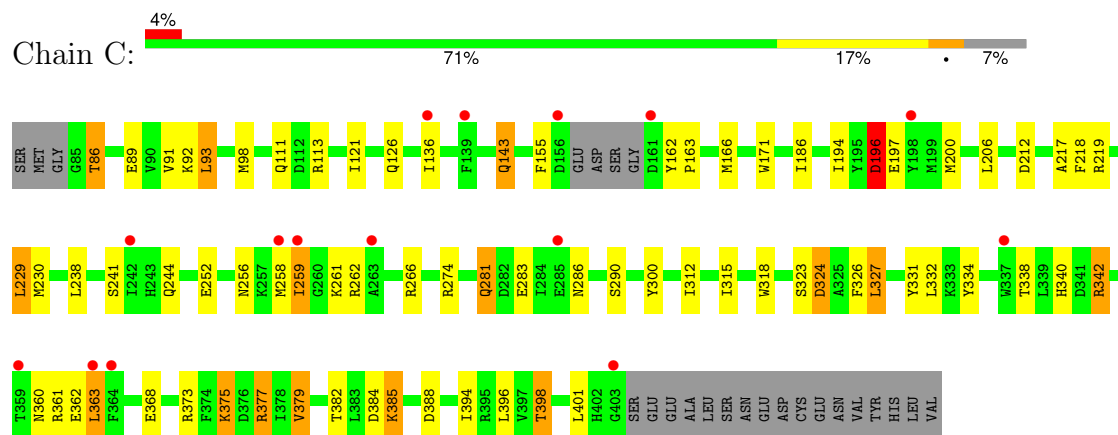
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	42	Total	O	0	0
			42	42		
3	A	37	Total	O	0	0
			37	37		
3	B	26	Total	O	0	0
			26	26		
3	D	52	Total	O	0	0
			52	52		

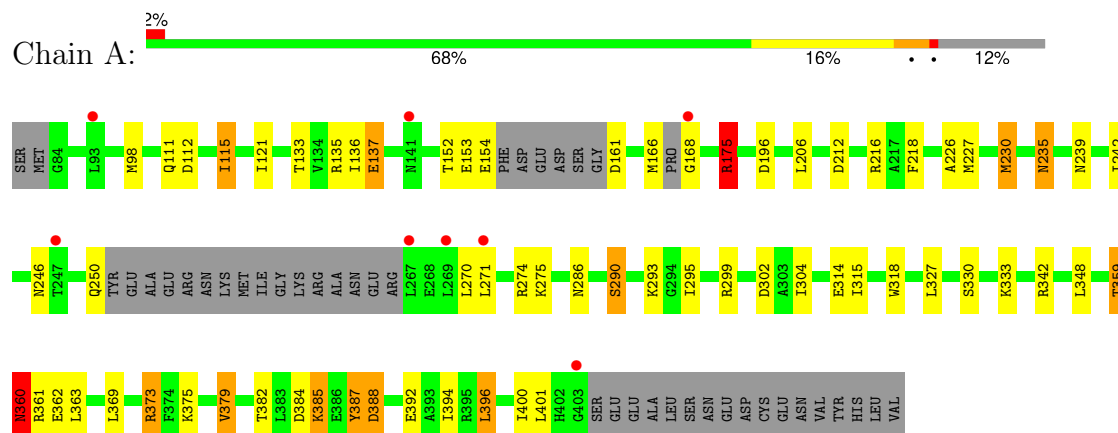
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

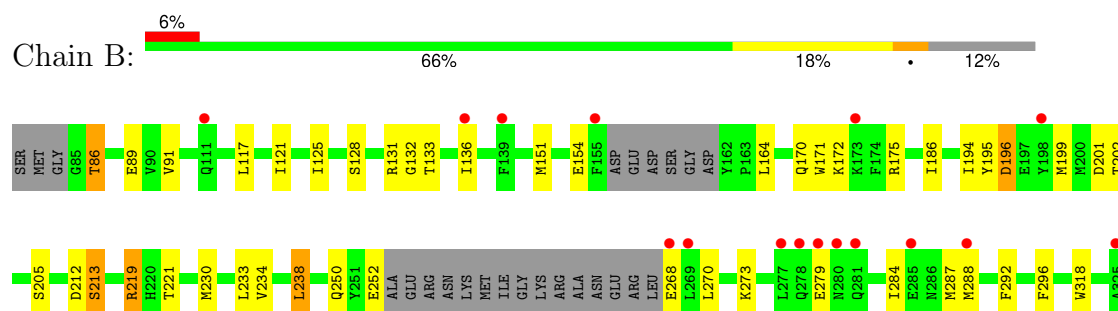
• Molecule 1: Cohesin subunit SA-1

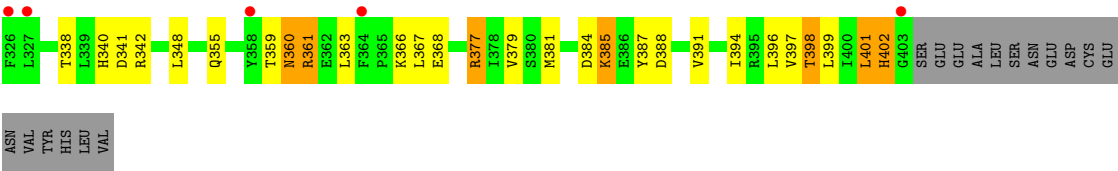


• Molecule 1: Cohesin subunit SA-1

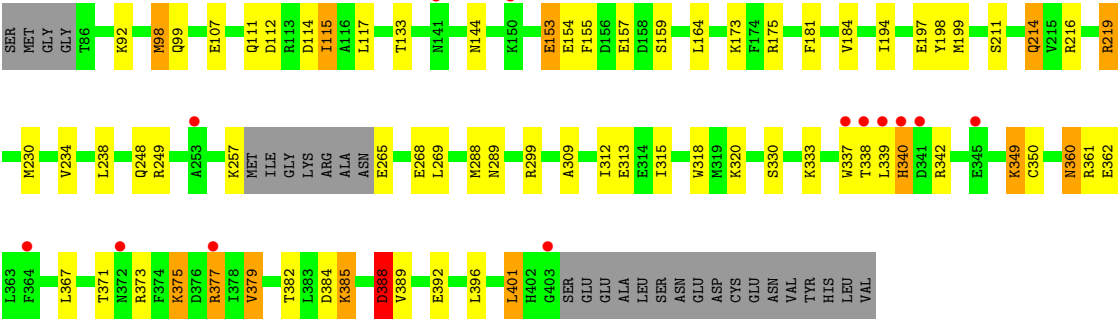


• Molecule 1: Cohesin subunit SA-1





• Molecule 1: Cohesin subunit SA-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.72Å 72.40Å 118.43Å 94.82° 98.37° 115.51°	Depositor
Resolution (Å)	115.57 – 2.34 115.57 – 2.34	Depositor EDS
% Data completeness (in resolution range)	96.4 (115.57-2.34) 96.4 (115.57-2.34)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.212 , 0.275 0.217 , 0.276	Depositor DCC
R_{free} test set	4078 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10244	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: O3M

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.74	0/2470	0.83	1/3319 (0.0%)
1	B	0.71	0/2493	0.84	0/3353
1	C	0.70	0/2629	0.84	1/3535 (0.0%)
1	D	0.69	0/2603	0.87	0/3501
All	All	0.71	0/10195	0.84	2/13708 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	C	196	ASP	CB-CA-C	5.79	121.98	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2433	0	2457	40	0
1	B	2452	0	2471	49	0
1	C	2587	0	2602	39	0
1	D	2561	0	2568	56	0
2	B	18	0	0	1	0
2	C	18	0	0	1	0
2	D	18	0	0	0	0
3	A	37	0	0	5	0
3	B	26	0	0	1	0
3	C	42	0	0	4	0
3	D	52	0	0	6	0
All	All	10244	0	10098	171	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:THR:HG22	1:D:350:CYS:SG	1.70	1.30
1:C:197:GLU:N	3:C:601:HOH:O	1.69	1.21
1:B:279:GLU:OE1	3:B:601:HOH:O	1.66	1.11
1:D:98:MET:SD	3:D:645:HOH:O	2.08	1.09
1:D:340:HIS:CE1	1:D:377:ARG:HG2	2.01	0.96
1:D:338:THR:CG2	1:D:350:CYS:SG	2.57	0.93
1:B:91:VAL:HG22	1:D:98:MET:CE	2.10	0.81
1:C:379:VAL:HG13	1:D:379:VAL:HG13	1.64	0.79
1:D:384:ASP:O	1:D:385:LYS:HB3	1.82	0.79
1:D:107:GLU:HG3	3:D:649:HOH:O	1.85	0.76
2:C:501:O3M:C13	2:C:501:O3M:C2	2.65	0.74
1:B:284:ILE:HG22	1:B:288:MET:HE3	1.69	0.74
1:B:384:ASP:O	1:B:385:LYS:HB2	1.88	0.73
1:B:91:VAL:HG22	1:D:98:MET:HE1	1.69	0.73
1:D:312:ILE:HG13	1:D:338:THR:HG21	1.69	0.73
1:D:340:HIS:CE1	1:D:377:ARG:CG	2.72	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:GLU:N	3:D:601:HOH:O	2.21	0.72
1:A:360:ASN:C	3:A:501:HOH:O	2.28	0.72
1:D:388:ASP:OD2	1:D:389:VAL:N	2.26	0.68
1:C:86:THR:HG21	3:A:532:HOH:O	1.96	0.66
1:B:230:MET:HG2	1:B:318:TRP:CZ2	2.31	0.66
1:C:384:ASP:O	1:C:385:LYS:HB2	1.96	0.65
1:D:248:GLN:HA	1:D:248:GLN:OE1	1.96	0.64
1:A:369:LEU:HD21	1:A:373:ARG:NH2	2.14	0.63
1:C:126:GLN:NE2	3:C:604:HOH:O	2.32	0.62
1:D:230:MET:HG2	1:D:318:TRP:CZ2	2.34	0.62
1:B:394:ILE:O	1:B:398:THR:HG22	2.00	0.62
1:D:384:ASP:O	1:D:385:LYS:CB	2.48	0.61
1:A:359:THR:O	1:A:360:ASN:HB2	2.01	0.61
1:D:234:VAL:HA	1:D:288:MET:CE	2.31	0.60
1:D:388:ASP:OD2	1:D:388:ASP:C	2.39	0.59
1:C:91:VAL:HG22	1:A:98:MET:HE1	1.83	0.59
1:D:112:ASP:HB3	1:D:115:ILE:HD12	1.84	0.59
1:D:360:ASN:HD21	1:D:362:GLU:HB2	1.67	0.59
1:C:162:TYR:CD1	1:C:217:ALA:HB2	2.38	0.58
1:C:340:HIS:CE1	1:C:377:ARG:HG3	2.39	0.58
1:B:284:ILE:HA	1:B:287:MET:CE	2.33	0.58
1:B:355:GLN:O	1:B:359:THR:HG23	2.03	0.57
1:C:384:ASP:O	1:C:385:LYS:CB	2.52	0.57
1:C:382:THR:OG1	1:D:379:VAL:CG2	2.52	0.57
1:B:230:MET:HG2	1:B:318:TRP:CE2	2.40	0.57
1:A:388:ASP:O	1:A:392:GLU:HG2	2.05	0.57
1:A:299:ARG:NH1	1:A:302:ASP:OD2	2.33	0.57
1:C:230:MET:HG2	1:C:318:TRP:CE2	2.40	0.56
1:B:128:SER:HA	1:B:221:THR:HG21	1.86	0.56
1:B:233:LEU:HB3	1:B:288:MET:HE2	1.88	0.55
1:D:153:GLU:O	1:D:155:PHE:N	2.39	0.55
1:C:143:GLN:HE21	1:C:143:GLN:HA	1.71	0.54
1:C:91:VAL:HG22	1:A:98:MET:CE	2.37	0.54
1:B:284:ILE:HD13	1:B:287:MET:HE2	1.89	0.54
1:B:360:ASN:C	1:B:361:ARG:O	2.46	0.54
1:B:86:THR:HG22	1:B:89:GLU:H	1.73	0.53
1:B:340:HIS:CE1	1:B:377:ARG:HG3	2.44	0.53
1:C:86:THR:HG22	1:C:89:GLU:H	1.73	0.53
1:C:375:LYS:O	1:C:379:VAL:HB	2.09	0.53
1:B:284:ILE:HG22	1:B:288:MET:CE	2.38	0.52
1:C:342:ARG:HD2	1:C:342:ARG:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:ARG:HD3	3:D:635:HOH:O	2.09	0.52
1:B:394:ILE:O	1:B:398:THR:CG2	2.57	0.52
1:D:360:ASN:C	1:D:360:ASN:HD22	2.12	0.52
1:D:114:ASP:OD1	1:D:198:TYR:OH	2.19	0.52
1:A:388:ASP:HB3	3:A:535:HOH:O	2.09	0.51
1:A:379:VAL:HG13	1:B:379:VAL:HG23	1.93	0.51
1:D:339:LEU:O	1:D:377:ARG:NH2	2.41	0.51
1:A:361:ARG:C	1:A:363:LEU:H	2.15	0.50
1:A:360:ASN:N	3:A:501:HOH:O	2.44	0.50
1:A:369:LEU:HD21	1:A:373:ARG:HH22	1.77	0.50
1:A:242:ILE:O	1:A:246:ASN:HB2	2.12	0.50
1:D:98:MET:HE2	1:D:181:PHE:HB2	1.94	0.49
1:B:91:VAL:HG13	1:D:98:MET:HE2	1.94	0.49
1:D:333:LYS:HD2	1:D:337:TRP:CH2	2.47	0.49
1:A:384:ASP:O	1:A:385:LYS:CB	2.60	0.49
1:D:98:MET:HG3	1:D:181:PHE:HA	1.95	0.49
1:D:330:SER:O	1:D:333:LYS:HE3	2.14	0.48
1:C:200:MET:HE1	1:C:229:LEU:HD21	1.96	0.48
1:C:274:ARG:HG3	3:C:613:HOH:O	2.11	0.48
1:A:361:ARG:HG3	3:A:501:HOH:O	2.12	0.48
1:D:211:SER:O	1:D:219:ARG:HG2	2.12	0.48
1:C:244:GLN:OE1	1:C:281:GLN:OE1	2.32	0.48
1:C:312:ILE:HG13	1:C:338:THR:HG21	1.94	0.48
1:A:166:MET:O	1:A:168:GLY:N	2.47	0.48
1:B:201:ASP:O	1:B:205:SER:HB2	2.13	0.48
1:B:284:ILE:HD13	1:B:287:MET:CE	2.44	0.48
1:B:171:TRP:CZ3	1:D:92:LYS:HD2	2.48	0.47
1:B:284:ILE:HA	1:B:287:MET:HE3	1.96	0.47
1:D:214:GLN:HA	1:D:214:GLN:HE21	1.78	0.47
1:C:327:LEU:CD1	1:C:332:LEU:HD11	2.45	0.47
1:D:164:LEU:CD2	1:D:175:ARG:HG3	2.44	0.47
1:A:216:ARG:CD	1:A:304:ILE:HG13	2.45	0.47
1:A:369:LEU:CD2	1:A:373:ARG:NH2	2.77	0.47
1:A:235:ASN:O	1:A:239:ASN:ND2	2.47	0.47
1:C:92:LYS:O	1:C:93:LEU:HB2	2.15	0.46
1:A:270:LEU:HD23	1:A:270:LEU:N	2.31	0.46
1:B:284:ILE:HA	1:B:287:MET:HE2	1.98	0.46
1:D:157:GLU:N	3:D:602:HOH:O	2.43	0.46
1:C:324:ASP:OD2	1:C:324:ASP:N	2.46	0.46
1:B:292:PHE:CE1	1:B:296:PHE:CD1	3.03	0.46
1:B:91:VAL:HA	1:D:98:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:THR:HB	1:B:397:VAL:HG11	1.98	0.46
1:C:194:ILE:HD11	1:C:200:MET:SD	2.57	0.45
1:A:286:ASN:O	1:A:290:SER:OG	2.34	0.45
1:B:117:LEU:O	1:B:121:ILE:HG12	2.16	0.45
1:D:333:LYS:CD	1:D:337:TRP:CH2	2.99	0.45
1:D:99:GLN:HA	1:D:184:VAL:HG11	1.99	0.45
1:A:175:ARG:HH11	1:A:175:ARG:HG3	1.82	0.45
1:C:394:ILE:O	1:C:398:THR:HG22	2.17	0.44
1:D:234:VAL:HA	1:D:288:MET:HE1	1.98	0.44
1:C:162:TYR:CD1	1:C:217:ALA:CB	2.99	0.44
1:A:327:LEU:CD2	1:A:363:LEU:HG	2.48	0.44
1:B:238:LEU:HD12	1:B:238:LEU:HA	1.87	0.44
1:D:401:LEU:HD23	1:D:401:LEU:HA	1.86	0.44
1:C:379:VAL:HG22	1:D:382:THR:OG1	2.18	0.44
1:B:213:SER:O	1:B:219:ARG:HD3	2.18	0.44
1:A:327:LEU:HD23	1:A:363:LEU:HG	1.99	0.44
1:B:250:GLN:HB3	1:B:270:LEU:HD11	1.99	0.44
1:D:315:ILE:HA	1:D:318:TRP:CE3	2.52	0.43
1:B:230:MET:O	1:B:234:VAL:HG23	2.18	0.43
1:C:196:ASP:C	3:C:601:HOH:O	2.30	0.43
1:C:315:ILE:HA	1:C:318:TRP:CE3	2.53	0.43
1:C:326:PHE:HA	1:C:331:TYR:HD2	1.84	0.43
1:C:379:VAL:CG1	1:D:379:VAL:HG13	2.42	0.43
1:B:125:ILE:CG2	1:B:132:GLY:HA3	2.49	0.43
1:B:384:ASP:O	1:B:385:LYS:CB	2.64	0.43
1:D:360:ASN:C	1:D:360:ASN:ND2	2.72	0.43
1:C:92:LYS:O	1:C:93:LEU:CB	2.67	0.43
1:B:151:MET:O	1:B:154:GLU:HB2	2.19	0.43
1:D:313:GLU:OE1	1:D:349:LYS:NZ	2.51	0.43
1:A:152:THR:O	1:A:154:GLU:N	2.52	0.43
1:A:360:ASN:HD22	1:A:360:ASN:HA	1.65	0.43
2:B:501:O3M:C5	2:B:501:O3M:C14	2.97	0.43
1:C:342:ARG:H	1:C:342:ARG:CD	2.31	0.42
1:B:387:TYR:O	1:B:391:VAL:HG23	2.19	0.42
1:D:342:ARG:NH1	3:D:607:HOH:O	2.52	0.42
1:C:186:ILE:HD13	1:C:229:LEU:HD23	2.02	0.42
1:A:394:ILE:HD12	1:B:401:LEU:HD12	2.01	0.42
1:B:121:ILE:HD11	1:B:202:THR:HG22	2.00	0.42
1:A:227:MET:HB3	1:A:314:GLU:HG2	2.01	0.42
1:D:309:ALA:HB1	1:D:349:LYS:HD3	2.00	0.42
1:A:315:ILE:HA	1:A:318:TRP:CE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:MET:HG2	1:C:318:TRP:CZ2	2.55	0.42
1:B:360:ASN:O	1:B:361:ARG:O	2.38	0.42
1:A:112:ASP:HB3	1:A:115:ILE:HD12	2.02	0.42
1:A:226:ALA:CB	1:A:295:ILE:HD13	2.49	0.42
1:B:196:ASP:OD1	1:B:196:ASP:C	2.58	0.42
1:D:371:THR:O	1:D:375:LYS:HB2	2.19	0.42
1:C:121:ILE:HG12	1:C:206:LEU:HD22	2.02	0.41
1:A:387:TYR:O	1:A:388:ASP:HB3	2.21	0.41
1:B:194:ILE:HG22	1:B:195:TYR:CD2	2.55	0.41
1:A:121:ILE:HD12	1:A:206:LEU:HD22	2.02	0.41
1:B:132:GLY:O	1:B:133:THR:HG23	2.20	0.41
1:A:135:ARG:NH1	1:A:137:GLU:OE2	2.46	0.41
1:A:226:ALA:HB2	1:A:295:ILE:HD13	2.01	0.41
1:C:163:PRO:HB3	1:C:171:TRP:CZ3	2.55	0.41
1:A:230:MET:HG2	1:A:318:TRP:CZ2	2.56	0.41
1:A:396:LEU:HD22	1:A:400:ILE:CD1	2.51	0.41
1:D:117:LEU:HD23	1:D:117:LEU:HA	1.89	0.41
1:C:360:ASN:ND2	1:C:363:LEU:HG	2.36	0.41
1:B:171:TRP:CH2	1:D:92:LYS:HD2	2.56	0.41
1:B:363:LEU:O	1:B:367:LEU:HD22	2.21	0.41
1:D:234:VAL:CA	1:D:288:MET:CE	2.98	0.41
1:D:249:ARG:NE	1:D:249:ARG:HA	2.36	0.41
1:B:164:LEU:HD23	1:B:164:LEU:HA	1.97	0.41
1:B:359:THR:HA	1:B:399:LEU:HD22	2.03	0.40
1:A:299:ARG:O	1:A:302:ASP:HB2	2.21	0.40
1:B:381:MET:O	1:B:384:ASP:HB2	2.22	0.40
1:D:388:ASP:O	1:D:392:GLU:HG2	2.21	0.40
1:A:387:TYR:O	1:A:388:ASP:CB	2.69	0.40
1:D:98:MET:CE	1:D:181:PHE:HB2	2.51	0.40
1:D:157:GLU:HA	1:D:159:SER:O	2.21	0.40
1:C:300:TYR:CZ	1:C:334:TYR:HD1	2.40	0.40
1:B:338:THR:O	1:B:341:ASP:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	289/339 (85%)	257 (89%)	27 (9%)	5 (2%)	7	5
1	B	292/339 (86%)	272 (93%)	16 (6%)	4 (1%)	9	7
1	C	311/339 (92%)	291 (94%)	14 (4%)	6 (2%)	6	4
1	D	307/339 (91%)	287 (94%)	16 (5%)	4 (1%)	10	8
All	All	1199/1356 (88%)	1107 (92%)	73 (6%)	19 (2%)	8	6

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	93	LEU
1	A	360	ASN
1	B	361	ARG
1	D	153	GLU
1	C	259	ILE
1	C	362	GLU
1	C	385	LYS
1	A	153	GLU
1	A	385	LYS
1	A	388	ASP
1	B	385	LYS
1	D	385	LYS
1	D	388	ASP
1	C	361	ARG
1	B	368	GLU
1	D	154	GLU
1	C	258	MET
1	B	402	HIS
1	A	387	TYR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/306 (88%)	240 (89%)	29 (11%)	5	4
1	B	271/306 (89%)	245 (90%)	26 (10%)	7	6
1	C	284/306 (93%)	245 (86%)	39 (14%)	3	2
1	D	283/306 (92%)	253 (89%)	30 (11%)	5	4
All	All	1107/1224 (90%)	983 (89%)	124 (11%)	5	4

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	86	THR
1	C	98	MET
1	C	111	GLN
1	C	113	ARG
1	C	136	ILE
1	C	143	GLN
1	C	155	PHE
1	C	166	MET
1	C	196	ASP
1	C	212	ASP
1	C	218	PHE
1	C	219	ARG
1	C	229	LEU
1	C	238	LEU
1	C	241	SER
1	C	252	GLU
1	C	256	ASN
1	C	259	ILE
1	C	261	LYS
1	C	262	ARG
1	C	266	ARG
1	C	281	GLN
1	C	283	GLU
1	C	286	ASN
1	C	290	SER
1	C	323	SER
1	C	324	ASP
1	C	327	LEU
1	C	342	ARG
1	C	363	LEU
1	C	368	GLU
1	C	373	ARG
1	C	375	LYS

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Mol	Chain	Res	Type
1	C	377	ARG
1	C	379	VAL
1	C	388	ASP
1	C	396	LEU
1	C	398	THR
1	C	401	LEU
1	A	111	GLN
1	A	115	ILE
1	A	133	THR
1	A	136	ILE
1	A	137	GLU
1	A	161	ASP
1	A	175	ARG
1	A	196	ASP
1	A	212	ASP
1	A	218	PHE
1	A	230	MET
1	A	235	ASN
1	A	250	GLN
1	A	271	LEU
1	A	274	ARG
1	A	275	LYS
1	A	290	SER
1	A	293	LYS
1	A	330	SER
1	A	333	LYS
1	A	342	ARG
1	A	348	LEU
1	A	360	ASN
1	A	362	GLU
1	A	373	ARG
1	A	375	LYS
1	A	379	VAL
1	A	396	LEU
1	A	401	LEU
1	B	86	THR
1	B	131	ARG
1	B	136	ILE
1	B	170	GLN
1	B	172	LYS
1	B	175	ARG
1	B	186	ILE

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Mol	Chain	Res	Type
1	B	196	ASP
1	B	199	MET
1	B	212	ASP
1	B	213	SER
1	B	219	ARG
1	B	238	LEU
1	B	252	GLU
1	B	268	GLU
1	B	273	LYS
1	B	342	ARG
1	B	348	LEU
1	B	360	ASN
1	B	366	LYS
1	B	377	ARG
1	B	388	ASP
1	B	396	LEU
1	B	398	THR
1	B	401	LEU
1	B	402	HIS
1	D	98	MET
1	D	111	GLN
1	D	115	ILE
1	D	133	THR
1	D	144	ASN
1	D	173	LYS
1	D	194	ILE
1	D	197	GLU
1	D	199	MET
1	D	214	GLN
1	D	219	ARG
1	D	238	LEU
1	D	257	LYS
1	D	268	GLU
1	D	269	LEU
1	D	289	ASN
1	D	299	ARG
1	D	320	LYS
1	D	340	HIS
1	D	349	LYS
1	D	360	ASN
1	D	361	ARG
1	D	367	LEU

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Mol	Chain	Res	Type
1	D	373	ARG
1	D	375	LYS
1	D	377	ARG
1	D	379	VAL
1	D	388	ASP
1	D	396	LEU
1	D	401	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	143	GLN
1	C	250	GLN
1	C	256	ASN
1	C	289	ASN
1	A	190	GLN
1	A	239	ASN
1	A	281	GLN
1	A	343	GLN
1	A	360	ASN
1	B	281	GLN
1	D	99	GLN
1	D	214	GLN
1	D	340	HIS
1	D	360	ASN
1	D	372	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	O3M	C	501	-	20,20,20	2.21	7 (35%)	27,27,27	1.93	8 (29%)
2	O3M	B	501	-	20,20,20	1.35	3 (15%)	27,27,27	1.32	5 (18%)
2	O3M	D	501	-	20,20,20	1.50	5 (25%)	27,27,27	1.81	8 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	O3M	C	501	-	-	0/4/13/13	0/3/3/3
2	O3M	B	501	-	-	0/4/13/13	0/3/3/3
2	O3M	D	501	-	-	0/4/13/13	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	O3M	C8-C7	-5.41	1.30	1.39
2	C	501	O3M	C12-C7	-4.19	1.32	1.40
2	C	501	O3M	C9-C8	-3.71	1.32	1.38
2	C	501	O3M	C10-C11	-3.35	1.33	1.38
2	C	501	O3M	C6-C7	-2.95	1.46	1.51
2	D	501	O3M	C4-C3	-2.75	1.46	1.51
2	B	501	O3M	C4-C3	-2.59	1.46	1.51
2	D	501	O3M	C5-C6	2.41	1.56	1.51
2	D	501	O3M	C4-N	2.34	1.52	1.47
2	C	501	O3M	C9-C10	-2.30	1.33	1.38
2	D	501	O3M	C13-N	2.15	1.50	1.47
2	C	501	O3M	C4-N	-2.14	1.43	1.47
2	B	501	O3M	C6-C7	-2.11	1.47	1.51
2	D	501	O3M	C5-N	2.05	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	O3M	C5-C6	2.01	1.55	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	O3M	C6-C5-N	-5.07	105.64	111.03
2	D	501	O3M	C6-C5-N	-4.48	106.27	111.03
2	C	501	O3M	C5-C6-C7	-3.46	105.36	111.34
2	D	501	O3M	C4-C3-C14	-3.35	114.58	120.75
2	C	501	O3M	C4-C3-C14	-2.83	115.53	120.75
2	D	501	O3M	C13-N-C5	2.77	113.90	110.03
2	B	501	O3M	C13-N-C5	-2.77	106.17	110.03
2	C	501	O3M	C2-C1-C	-2.69	117.03	119.88
2	D	501	O3M	C4-N-C13	-2.68	106.98	111.57
2	C	501	O3M	C12-C13-N	2.64	115.18	112.14
2	D	501	O3M	C2-C3-C14	2.57	122.06	118.23
2	C	501	O3M	C4-N-C5	-2.57	105.53	111.07
2	B	501	O3M	C5-C6-C7	-2.48	107.05	111.34
2	B	501	O3M	C6-C5-N	-2.45	108.43	111.03
2	B	501	O3M	C3-C4-N	-2.26	108.53	113.15
2	D	501	O3M	C2-C1-C	-2.23	117.52	119.88
2	D	501	O3M	C3-C4-N	2.21	117.67	113.15
2	C	501	O3M	C4-N-C13	-2.21	107.79	111.57
2	B	501	O3M	C4-N-C5	-2.14	106.46	111.07
2	C	501	O3M	C6-C7-C12	-2.04	116.42	120.77
2	D	501	O3M	C11-C12-C7	2.01	121.45	118.98

There are no chirality outliers.

There are no torsion outliers.

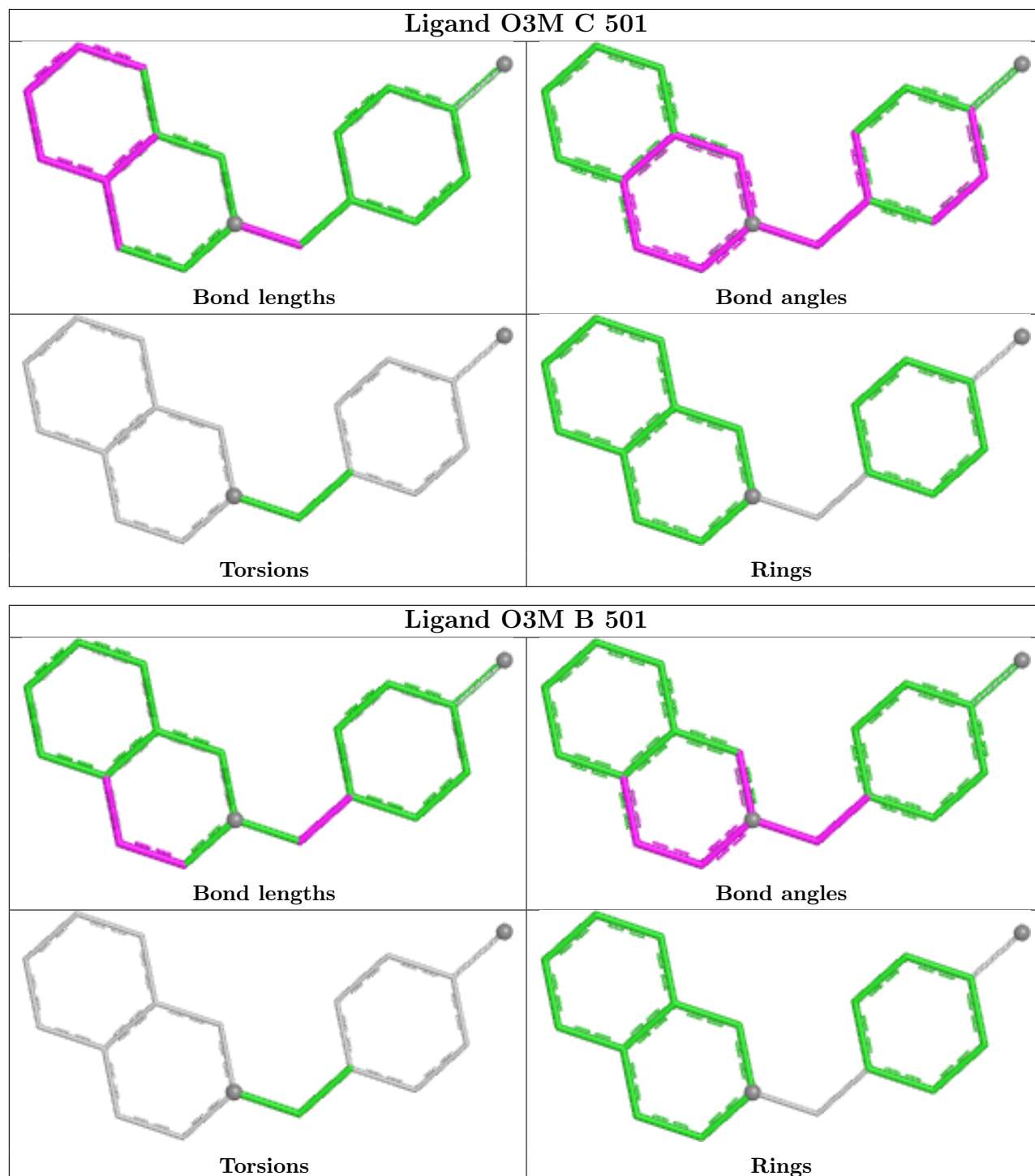
There are no ring outliers.

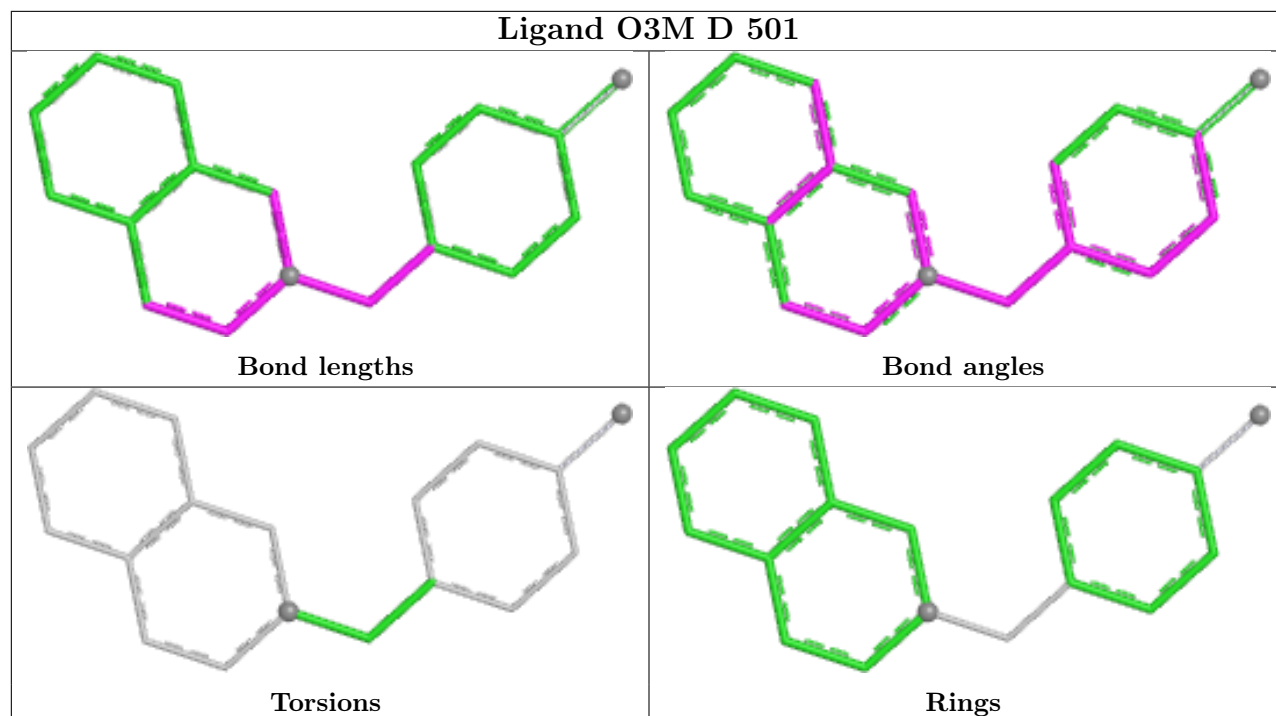
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	O3M	1	0
2	B	501	O3M	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	297/339 (87%)	0.43	8 (2%) 56 62	59, 85, 136, 187	0
1	B	298/339 (87%)	0.59	21 (7%) 24 30	20, 78, 124, 147	10 (3%)
1	C	315/339 (92%)	0.34	15 (4%) 36 44	22, 77, 122, 163	1 (0%)
1	D	311/339 (91%)	0.40	13 (4%) 41 48	13, 70, 120, 161	6 (1%)
All	All	1221/1356 (90%)	0.44	57 (4%) 37 44	13, 78, 125, 187	17 (1%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	337	TRP	14.2
1	D	339	LEU	13.6
1	D	340	HIS	12.8
1	D	341	ASP	11.9
1	B	326	PHE	11.6
1	D	338	THR	11.5
1	C	285	GLU	11.3
1	D	377	ARG	10.0
1	B	281	GLN	9.9
1	B	279	GLU	9.0
1	B	325	ALA	8.9
1	B	277	LEU	8.8
1	B	278	GLN	7.9
1	B	285	GLU	7.9
1	B	288	MET	7.0
1	B	280	ASN	6.8
1	B	139	PHE	6.2
1	B	327	LEU	4.8
1	B	136	ILE	4.7
1	A	269	LEU	4.4
1	C	403	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	155	PHE	3.8
1	B	403	GLY	3.7
1	D	403	GLY	3.6
1	A	403	GLY	3.6
1	B	198	TYR	3.6
1	C	263	ALA	3.3
1	C	139	PHE	3.1
1	D	372	ASN	3.0
1	C	198	TYR	3.0
1	D	253	ALA	3.0
1	C	259	ILE	2.9
1	D	141	ASN	2.9
1	A	168	GLY	2.7
1	A	141	ASN	2.7
1	C	161	ASP	2.7
1	B	269	LEU	2.7
1	A	247	THR	2.6
1	A	271	LEU	2.5
1	C	364	PHE	2.4
1	A	267	LEU	2.4
1	B	111	GLN	2.4
1	B	268	GLU	2.4
1	D	345	GLU	2.4
1	D	364	PHE	2.4
1	C	337	TRP	2.3
1	B	364	PHE	2.3
1	C	258	MET	2.3
1	D	150	LYS	2.2
1	C	363	LEU	2.2
1	C	242	ILE	2.1
1	A	93	LEU	2.1
1	C	359	THR	2.1
1	B	358	TYR	2.1
1	C	156	ASP	2.1
1	C	136	ILE	2.0
1	B	173	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

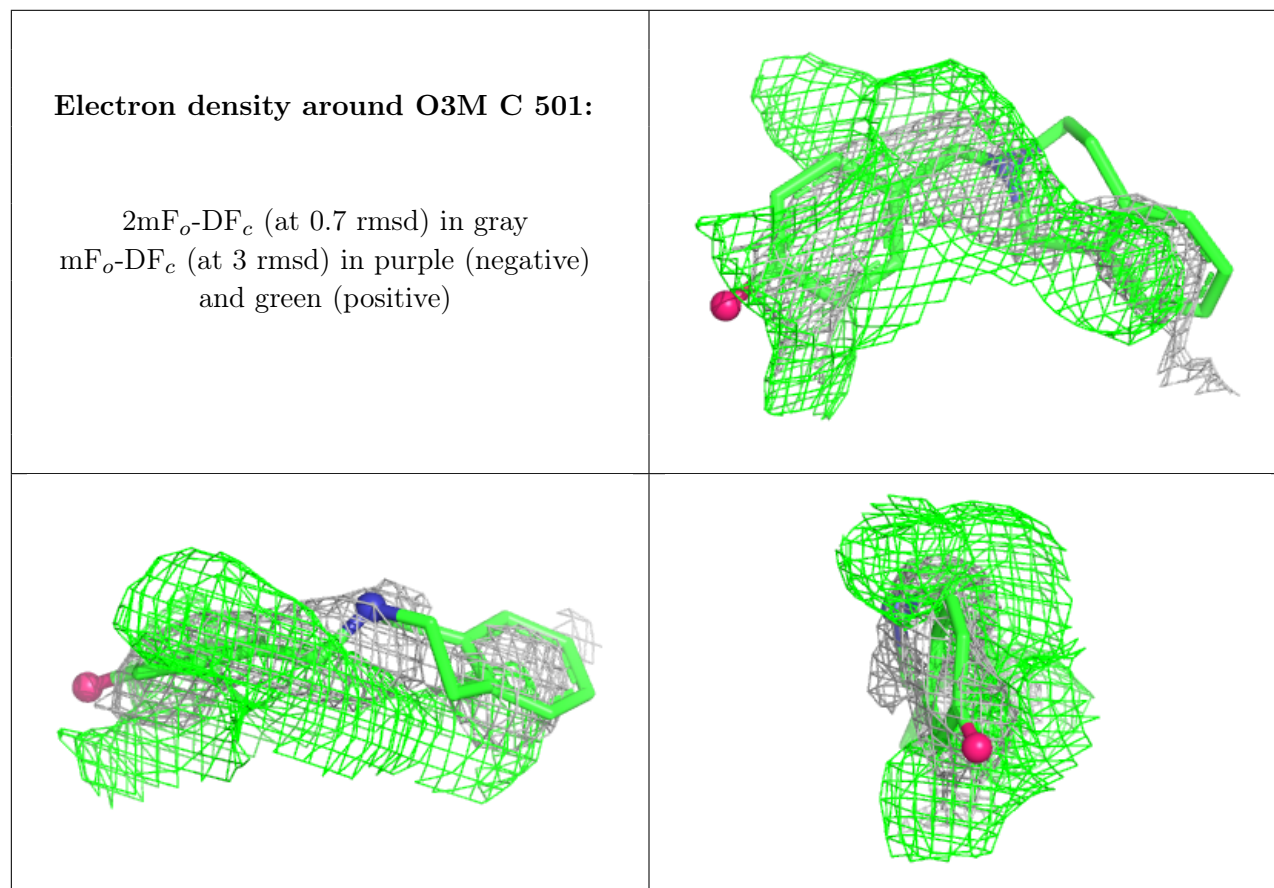
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

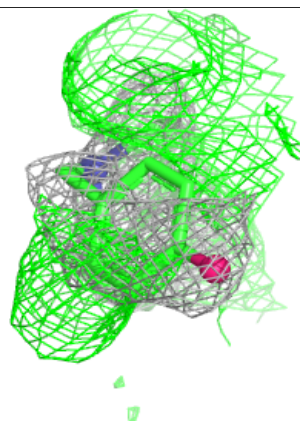
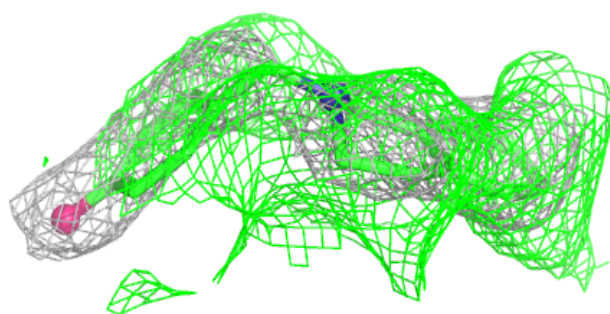
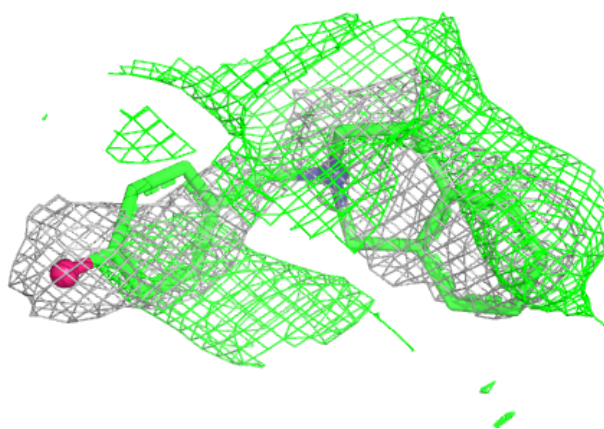
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	O3M	C	501	18/18	0.85	0.45	58,68,79,83	18
2	O3M	D	501	18/18	0.90	0.29	41,48,55,56	18
2	O3M	B	501	18/18	0.92	0.26	48,54,66,72	18

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

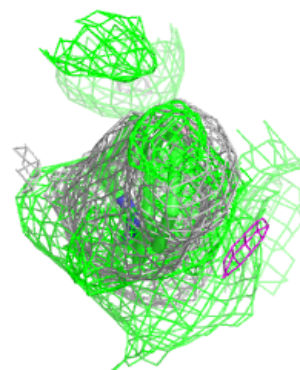
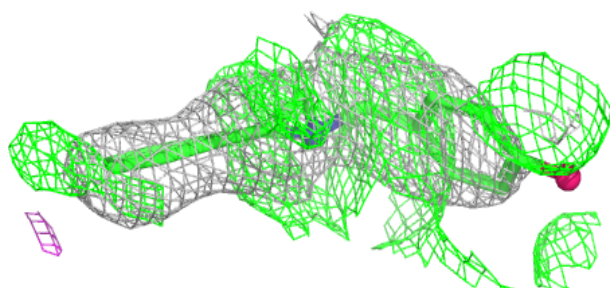
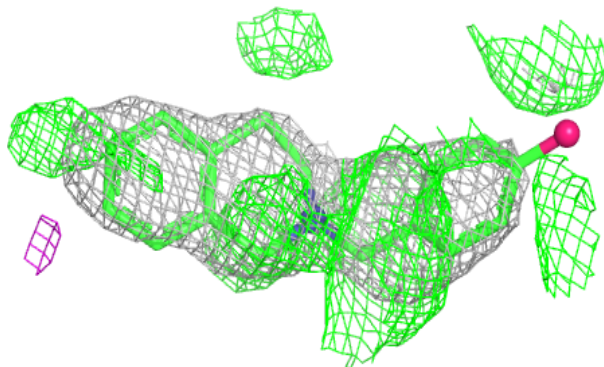


Electron density around O3M D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around O3M B 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.